

Use of CAPE-OPEN Standard in US-UK Collaboration on Virtual Plant Simulation

Stephen E. Zitney

Collaboratory for Process & Dynamic Systems Research
National Energy Technology Laboratory, Morgantown, WV 26507-0880
stephen.zitney@netl.doe.gov www.netl.doe.gov

Under the auspices of a US-UK Memorandum of Understanding and Implementing Agreement for fossil energy R&D (<http://us-uk.fossil.energy.gov/>), the US Department of Energy's (DOE) National Energy Technology Laboratory (NETL) and the UK Department of Trade and Industry (DTI) have recently completed a three-year collaboration on virtual plant modeling and simulation technology for advanced fossil-energy power generation systems. The R&D collaboration was aimed at taking full advantage of the synergies between NETL's ongoing Advanced Process Engineering Co-Simulator (APECS) project and the UK's three-year Virtual Plant Demonstration Model (VPDM) project. The key objective of this collaboration has been the development of compatible, open standards-based US and UK technology for process/equipment co-simulation. To achieve plug-and-play model interoperability, the collaboration leveraged the process-industry CAPE-OPEN (CO) software standard which is managed and disseminated by the CO Laboratories Network (www.colan.org).

We highlight here the use of the CO interfaces for facilitating the interoperability of power plant equipment models between the APECS and VPDM software platforms. Special emphasis will be focused on the use of the CO steady-state unit operation interfaces to integrate process simulation with a hierarchy of equipment models ranging from computational fluid dynamics (CFD) models to fast reduced-order models (ROMs) based on CFD results. Virtual plant simulations based on CO compliant process/CFD co-simulations will accelerate the design of next-generation plants to operate with unprecedented efficiency and near-zero emissions, while operating profitably amid cost fluctuations for raw materials, finished products, and energy.

APECS

NETL's **Advanced Process Engineering Co-Simulator (APECS)** system is an integrated software suite that combines process simulation, high-fidelity CFD, immersive and interactive 3D plant walk-through virtual engineering, and advanced analysis capabilities including case studies, sensitivity analysis, stochastic simulation for risk/uncertainty analysis, and multi-objective optimization. To facilitate effective technology transfer, the APECS system was designed using commercial process simulation and CFD software with model interoperability provided by the CAPE-OPEN interfaces for unit operations, physical properties, and reaction kinetics.

Using APECS, design engineers can effectively integrate and efficiently solve and analyze co-simulations combining the CO-compliant, steady-state process simulators such as Aspen Plus® (www.aspentech.com), Aspen HYSYS®, and gPROMS® (www.psenterprise.com) with CO-compliant process equipment models, including CFD models based on FLUENT® (www.fluent.com), the world's leading software for detailed flow analysis of process equipment. APECS also offers fast ROMs based on pre-computed CFD solutions over a range of parameter values. For example, the APECS system currently provides for automatically generating and using ROMs based on multiple linear regression and neural networks. Future ROM solvers will include principal component analysis (PCA) and proper orthogonal decomposition (POD). The CAPE-OPEN COM/CORBA bridge implementation in APECS allows process simulations running under the Windows operating system to use equipment models running locally/remotely and serially/in parallel on Linux clusters and/or supercomputers.

Advanced 2D and 3D visualization tools, including Paraview (www.paraview.org), available in APECS enable design engineers to display, within the process simulator, the results of a process/CFD co-simulation including contours of velocity, temperature, pressure, and species mass fractions for specified surfaces in the equipment models. Ongoing collaborative efforts aimed at integrating APECS with VE-Suite (www.vesuite.org), an open-source virtual engineering software toolkit, will enable users to explore

co-simulation results in a context-based, user-centered interface including walking through a 3D representation of the power plant.

The APECS system also provides a wide variety of powerful analysis tools for optimizing overall power plant performance. Optimization is used for maximizing an objective function, including plant efficiency, energy production, and process economics. For process optimization in the face of uncertain variables and multiple and some time conflicting objectives, APECS offers stochastic modeling and multi-objective optimization capabilities developed to comply with the CO software standard.

In March, 2005, U.S. Secretary of Energy, Samuel Bodman, announced that Ansys/Fluent (www.ansys.com) and Reaction Engineering International (www.reaction-eng.com) were awarded APECS projects, respectively, as part of a portfolio of 32 clean coal research projects. These phase-II APECS software development projects are well underway and have been augmented recently with a portfolio of APECS R&D projects launched under the auspices of NETL's Collaboratory for Process & Dynamic Systems Research organized in partnership with Carnegie Mellon University, the University of Pittsburgh, and West Virginia University.

At NETL, system analysts are applying APECS to a wide variety of advanced power generation systems, ranging from small fuel cell systems to commercial-scale power plants. Using APECS, the overall performance of solid oxide fuel cell (SOFC) auxiliary power units (APUs) system modeled using Aspen Plus are optimized with respect to the local fluid flow, heat and mass transfer, electrochemical reactions, current transport, and potential field in the SOFC simulated using detailed, three-dimensional, steady-state FLUENT CFD models. The process/CFD co-simulations are performed over a range of fuel cell currents to generate a voltage-current curve and analyze the effect of current on fuel utilization, power density, and overall system efficiency.

In collaboration with cycle engineers at Alstom Power (www.power.alstom.com), APECS co-simulations have been developed for a conventional 30 MWe pulverized coal-fired (PC) steam plant for municipal electricity generation and an advanced 250 MW, natural gas-fired, combined cycle (NGCC) power plant. In the PC co-simulation, an Aspen Plus process design specification is used to adjust a FLUENT CFD model parameter for the boiler damper position (bypass resistance) to maintain a specified steam temperature over a range of loads, from the load at the maximum continuous rating to a control load, below which the boiler cannot sustain the required turbine inlet temperatures. For the NGCC co-simulation, an Aspen Plus process design specification is used to manipulate designated control parameters for the FLUENT CFD model of the heat recovery steam generator (HRSG) so that a specified superheat steam temperature is maintained for various load points over the range from 100% to 50% gas turbine load.

At NETL, research engineers are also developing APECS co-simulations to analyze potential FutureGen plant configurations. The DOE's 10-year, FutureGen Research Initiative is aimed at creating the world's first coal-based, near-zero emissions electricity and hydrogen production power plant with carbon capture and storage (www.futuregenalliance.org). In a recent demonstration case, the FutureGen co-simulation combines a plant-wide Aspen Plus simulation with two FLUENT CFD-based equipment models, one for the entrained-flow gasifier where fluid dynamics strongly affect syngas quality and carbon conversion and one for the gas turbine combustor where the blending of air and fuel is at the heart of gas turbine combustor performance and efficiency. Using APECS, Aspen Plus controls the co-simulation and automatically executes the gasifier and combustor CFD models as needed to converge the tail gas recycle loop and a design specification on the gas turbine inlet temperature. The design specification is met by manipulating the synthesis gas split between power production and hydrogen production.

The co-simulation applications described here illustrate how APECS is helping engineers optimize the coupled fluid flow, heat and mass transfer, and related phenomena that drive overall system performance. By combining process simulation and CFD software, together with advanced visualization and high-performance computing, APECS provides the high-fidelity solution and analysis capabilities required to achieve the aggressive integration, environmental, and performance goals for advanced power generation systems such as the DOE's FutureGen plant.

VPDM

The principal objective of the UK's **Virtual Plant Demonstration Model (VPDM)** project was to develop a software framework for accurate power plant modelling. The project had participants from UK companies and academia, and received support from the DTI Carbon Abatement Technologies Programme. The partners included: ALSTOM Power Ltd., Engineous Software Ltd., Ansys Fluent Europe Ltd., RWE npower plc, K-S Tech Ltd., Doosan Babcock Energy Ltd., Process Systems Enterprise Ltd. (PSE), and the University of Ulster. The concept of the VPDM is that it is able to utilize the most accurate plant equipment models available, many of which are proprietary and residing on various hardware platforms at different locations. The VPDM team leveraged NETL's APECS technology to integrate high-fidelity FLUENT CFD equipment models into overall power plant simulations developed with PSE's gPROMS simulator. The project also exploited the common standards for interfacing based on the CAPE-OPEN standard. In the development of the VPDM, the following CO-compliant process simulators were tested: gPROMS from PSE, Aspen Plus from Aspen Technology, and ECLIPSE from the University of Ulster.

Another key feature of the VPDM process modeling environment is that it allows secure web interfacing and data exchange with individual heterogeneous component models located remotely at partner sites. Thus, companies can allow access to their in-house equipment models without compromising the intellectual property contained within the models. The VPDM framework and the availability of such models will provide the opportunity to investigate, through simulation studies, accurate novel power plant solutions which are capable of producing power in a reliable, cost-effective and environmentally friendly manner. The proposed VPDM framework uses the web technology contained within FIPER from Engineous (www.engineous.com) to provide a secure client-server communications layer between partner companies over the Internet. Some special software developed by PSE and Engineous, as part of the VPDM program, enables FIPER to communicate with CO-compliant process simulators and CO-compliant equipment models.

The initial target application for the VPDM was the simulation of a 500 MW conventional coal-fired power plant. Using CO-based process/CFD co-simulation technology in NETL's APECS system, the VPDM team coupled a detailed FLUENT CFD furnace simulation with a steady-state gPROMS process simulation of the power plant. As a demonstration of the VPDM's versatility, it was also successfully applied to two new fossil power plant technologies which both include carbon capture.

US-UK Collaboration Tasks

Joint APECS/VPDM work began in January 2005 on four key collaborative tasks which are outlined below.

Collaboration Task 1: Using CAPE-OPEN Interface for Interoperability of Equipment Component Models and Virtual Power Plant Simulation Frameworks

The objective of this collaboration task was the exchange of information and experience in the development and application of CO-compliant equipment models based on the FLUENT CFD code for use in the UK and US projects. The following benefits were achieved:

- Developed plug-and-play capability, between US equipment component models and the VPDM framework, as well as between UK equipment models and NETL's APECS simulation frameworks.
- Placed initial emphasis on using FLUENT CFD models within both software environments.
- Focused on using the process industry standard CO interfaces.

Collaboration Task 2: Using Reduced-Order Component Models to Enhance Speed of CFD models for Virtual Power Plant Simulation Frameworks

A potential barrier to the widespread use of process/CFD co-simulation is that the integration of high-fidelity equipment models may lead to unacceptable co-simulation turnaround times, especially for cases in which one or more CFD models are embedded in the iterative flowsheet solution process. One promising solution is the use of reduced-order models (ROMs) that approximate the CFD-based equipment

simulations, while keeping the computational cost manageable. The key benefits of this collaboration task were the following:

- Allowed US DOE/NETL and UK (PSE) researchers to collaborate in their evaluation of order reduction techniques for application to power plant simulation.
- Collaborated to devise strategies for implementing order reduction techniques in respective UK and US programs.
- Exchanged information on accuracy and speed of ROMs as implemented in the simulators.

Collaboration Task 3: Internet Security and Communication

The fundamental aim of both the UK's and the US's projects is to obtain maximum accuracy from power plant simulation models by linking together existing plant component models that have benefited from many years of development, validation, and refinement. These models contain propriety information and each model owner will want to operate their model from their own site, where they have confidence that their know-how is secure. The main benefit of this collaboration task was the exchange of information to determine the specification of security requirements suitable for users of the simulation frameworks.

Collaboration Task 4: CAPE-OPEN Dynamic Simulation

Both the US and UK virtual power plant simulation programs are planning to pursue dynamic simulation, especially for use in process control. The process industry-standard CO interfaces currently support steady-state modelling only, but a standard for dynamic modelling is under development. The benefits of this collaboration task were as follows:

- Reviewed current status of CO dynamic simulation standard.
- Identified the dynamic modelling requirements of the APECS and VPDM projects.
- Worked with the CO developers to ensure that the CO interfaces for dynamic simulation are developed in a timely manner and meet the agreed requirements of the VPDM and APECS projects.

Collaboration Benefits

The US-UK collaboration has worked well; in particular the joint adoption of the CAPE-OPEN software standard will have benefits on both sides of the Atlantic and allow interoperability between equipment models in the US APECS project and UK VPDM project. The US project is currently focusing on using FLUENT to create appropriate CFD-based models for advanced power plants and these models will be run with the Aspen Plus process simulator. The success of this collaboration task means that it will be possible to use these CFD models with the VPDM framework. Similarly, the UK FLUENT based CFD models can be used in the US APECS system. The exchange of ideas and information on Internet security and protecting IP has resulted in an organization external to the VPDM project approving of the techniques used in the VPDM; this gives confidence for the future adoption of the VPDM principals beyond the VPDM project.

By leveraging the US APECS project, UK VPDM project, and the international process-industry CAPE-OPEN software standardization effort, the US-UK collaboration on virtual power plant simulation achieved its main goal which was to develop compatible process/CFD co-simulation software platforms for application to advanced fossil energy systems. The key benefits to US and UK fossil energy industries include:

- Helps engineers to better understand and visualize the fluid flow behavior that impacts process design and operation
- Considers detailed equipment models in the context of plant-wide simulations, with recycle loops, heat integration, and water management
- Enables rigorous analysis and optimization of entire plants with respect to CFD-related equipment model parameters

- Eliminates potential for suboptimal designs by using same physical properties and reaction kinetics in the underlying equipment and process models
- Speeds technology development by reducing pilot/demo-scale facility design time and operating campaigns
- Offers opportunities to achieve the aggressive environmental, performance, and economic goals for high-efficiency, zero-emission power plants

Continued US-UK collaboration on virtual power simulation will accelerate the development of competitive power plant solutions and ultimately zero-emission technologies with significantly reduced development costs and technical risk.